chapter 4

Survival analysis applied to sensory shelf life

4.1 What is survival analysis?

Generally, survival analysis is a collection of statistical procedures for data analysis for which the outcome variable of interest is time until an event occurs (Kleinbaum 1996). The problem of analyzing time to event data arises in a number of applied fields, such as medicine, biology, public health, epidemiology, engineering, economics, and demography (Klein and Moeschberger 1997). Following is a series of examples of how time to an event of interest is considered (Gómez and Langohr 2002):

- In a clinical trial of a certain medicine, time zero is when patients are randomly allocated to treatments. Time to event is the time till cancer remission or time till a clinical indicator falls below a certain level, for example, viral count falls below 500.
- In an epidemiological study the event of interest could be the weaning of newborn baby. Time zero is the birth of the child, and time to the event is the last day the baby breastfeeds.
- Another epidemiological study could measure the time from when a person starts consuming intravenous drugs until infection with the HIV virus.
- In industrial durability tests it is of interest to know, for example, how long a car tire lasts. In this case, instead of *time to event*, *kilometers to event* is used. That is, instead of recording the time the tire is on the road, the distance in kilometers run by the car till the tire wears out is recorded.
- In a psychological study it is of interest to know, for example, the time it takes 2-year old children to learn a certain task.
- In a sociological study the event of interest could be returning to jail after having left jail for the first time. That is, the time to event would be measured from when the person was let out of jail for the first time till the person returns due to a new offence.
- In a SSL, time to event would be measured from when the product left the manufacturing plant till it was rejected by a consumer (Hough et al. 2003).

4.2 Censoring

Time-to-event data present themselves in different ways, which creates special problems in analyzing such data. One feature, often present in time-to-event data, is known as *censoring*, which, broadly speaking, occurs when some lifetimes are known to have occurred only within certain intervals. There are three basic categories of censoring: right-, left-, and interval-censored data.

4.2.1 Right-censoring

Subjects are followed till the event of interest occurs. If the event of interest does not occur during the period the subject is under study, this observation is right-censored. Continuing the above examples, this type of censoring can occur:

At the end of the study
- A cancer patient is still alive
- A tire has not worn out
- A 2-year old child is still breastfeeding
- An ex-prisoner has not returned to jail
- A consumer still accepts the sample stored for the maximum time

In the middle of a study
- A patient moves and leaves no forwarding address
- A tire bursts for extraneous reasons
- A consumer no longer wants to taste samples stored for successive times

In all these cases the event had not occurred up to a certain time, and this information is used in modeling the data.

4.2.2 Left-censoring

Left-censoring occurs if the subject has already undergone the event of interest before the study begins. Following are three examples of left-censored data:

- In a study on the aroma persistence of a clothes rinse, standard-sized hand towels are washed using the rinse, tumble dried, and kept in a cupboard. At different times after the application, respondents sniff a smelling strip with the aroma of the clothes rinse and are then asked if they can definitely detect the aroma on the towel. Suppose that

the first test is 24 hours after the application. If a respondent cannot detect the aroma at this first test, then his data are left-censored. For this respondent, the aroma disappeared sometime between Time = 0 (application) and Time = 24 hours (first test).

- For a study to determine the distribution of the time until first marijuana use among high school students (Klein and Moeschberger 1997), the question "When did you first use marijuana?" was asked. One of the responses was, "I have used it but cannot recall just when the time was." A boy who chose this response is indicating that the event occurred prior to age at interview, but the exact age at which he started using marijuana is unknown. His data is left-censored.
- In an SSL study on mayonnaise it would not be necessary to ask consumers to taste samples with less than 2 months' storage at 25°C. If a consumer rejects a sample with 2 months' storage because she is particularly sensitive to oxidized flavor, her data are left-censored. That is, all that is known is that time to rejection for this consumer lies somewhere between Time = 0 and Time = 2 months.

4.2.3 Interval-censoring

Interval-censoring occurs when all that is known is that the event of interest occurred within a time interval. Following are two examples of interval-censored data:

- Longitudinal epidemiological studies are likely to have interval-censored data. For example, populations who consume intravenous drugs are highly vulnerable to infection with the HIV virus. It could be of interest to estimate the distribution of times between first intravenous drug consumption and infection with HIV. To do this, periodic blood tests are taken on willing participants. A protocol is agreed with each volunteer, for example, to perform a test every 6 months. If the HIV test was negative on June 1 but is positive on December 1, then what is known is that the subject became infected sometime between these two dates. If the subject skips a test, and the positive test is only detected on June 1 of the following year, then the infection interval is extended to 12 months.
- In SSL tests, interval-censoring is very likely to occur. In a study on the SSL of cracker-type biscuits, the maximum storage time at 20°C and 60% relative humidity is considered to be 12 months. If a reversed storage design is used (see Section 3.3.6.2), samples with different storage times are presented to consumers in a single session. To know the exact storage time at which a consumer will reject the crackers, samples would have to be taken on a daily basis. Obviously, this is not possible. Over the 12-month period, suppose that the

following storage times are chosen: 0, 3, 6, 8, 10, and 12 months. If a consumer accepts the sample with 6 months' storage and rejects the sample with 8 months' storage, what is known is that her rejection time is somewhere between 6 and 8 months' storage. Her data are thus interval-censored.

In actual fact, both right-censored and left-censored data can be considered as special cases of interval-censoring. For an SSL study, with right-censored data the interval is between the last time the consumer accepted the sample and infinity, and with left-censored data the interval is between Time = 0 and the first storage time.

4.3 Survival and failure functions

Let T be the time of occurrence of event ε. Event ε could be death, appearance of a tumor, giving up smoking, end of itching symptoms, or a projector lamp burning out. For SSL studies, event ε is rejection of a stored product by the consumer. T is a random non-negative variable whose distribution can be characterized by the following functions:

- Survival function, $S(t)$
- Failure function (also referred to as cumulative distribution function), $F(t)$
- Probability density function, $f(t)$
- Hazard function, $h(t)$

If any of these functions is known, the others can be determined univocally. We will define the survival and failure functions.

The survival or acceptance function is the probability of an individual surviving beyond time t: $S(t) = \text{Prob}(T > t)$ and is defined for $t \geq 0$. In SSL the survival function is the probability of a consumer accepting a food product stored beyond time t and is thus referred to as the acceptance function. Figure 4.1 shows a typical survival, or acceptance, curve. Its basic properties are as follows:

- $S(0) = 1$: the consumer accepts the fresh product
- $S(\infty) = 0$: the consumer rejects the product stored for prolonged periods
- $S(t)$ is a monotonously decreasing function
- If T is continuous, $S(t)$ is continuous and strictly decreasing

The failure or rejection function (also known as cumulative distribution function of T) is the probability of an individual failing before time t: $F(t) = \text{Prob}(T \leq t)$ and is defined for $t \geq 0$. In SSL the rejection function is the probability of a consumer rejecting a food product stored for less than

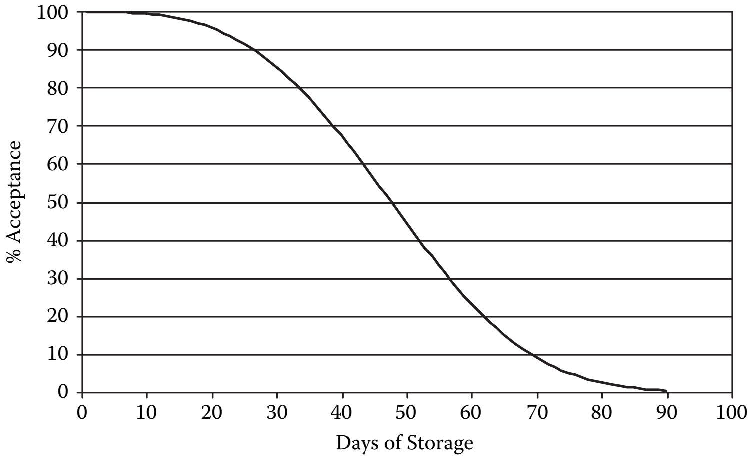

Figure 4.1 Survival or acceptance function.

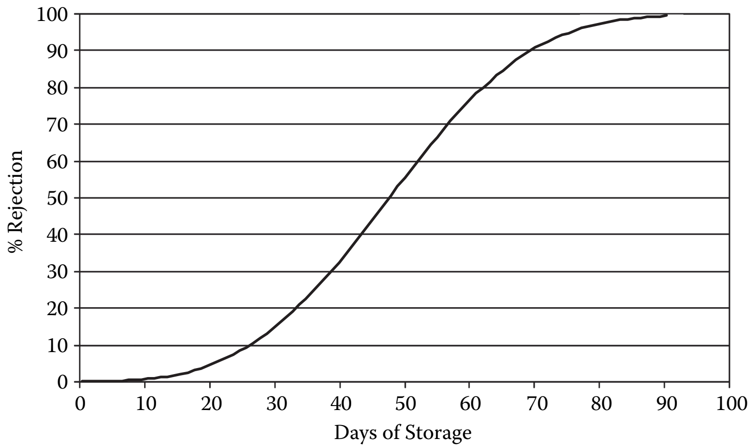

Figure 4.2 Failure or rejection function.

time t. It can also be interpreted as the proportion of consumers who will reject a food product stored for less than time t. Figure 4.2 shows a typical failure or rejection curve.
Its basic properties are as follows:

- F(0) = 0: the consumer accepts the fresh product
- F(∞) = 1: the consumer rejects the product stored for prolonged periods
- F(t) is a monotonously increasing function
- If T is continuous, F(t) is continuous and strictly increasing
- F(t) = 1 − S(t)

4.4 Shelf life centered on the product or on its interaction with the consumer?

Chapter 1 (Section 1.3) pointed out that the first step in establishing the shelf life of a product is to make sure consumers will come to no harm through eating the food during the established storage time. For some foods the nutrition aspect is crucial. Once the sanitary and nutritional hurdles have been overcome, the remaining barrier depends on the sensory properties of the product.

There are numerous examples in the food science literature where the SSL is centered on the product. For example, Fan et al. (2003) studied the use of ionizing radiation to extend the SSL of fresh-cut green onion leaves. Three assessors measured the overall quality of the onion leaves using a scale of 1 (*non-eatable*) to 9 (*excellent*). The authors decided that a value of 6 on this scale was the commercialization limit. They established that the SSL of the product was 9 days. This is what we call centering the shelf life on the product. It would be interesting to know what the consumers think about these onion leaves stored for 9 days. A very sensitive or fussy consumer would very probably find the product stored for 6 days totally unacceptable. On the other hand a less sensitive or less fussy consumer would probably be quite happy consuming onion leaves with 12 days storage. That is, from a sensory point of view, the onion leaves do not have a shelf life of their own; rather, this will depend on the interaction of the product with the consumer. The same onion leaves can be accepted by some consumers and rejected by others.

Another example was a study reported by Martínez et al. (2005) on the use of modified atmospheres to extend the shelf life of pork sausages. A six-member panel measured appearance and off-odor. For off-odor a 5-point scale was used, where 1 = *none* and 5 = *extreme*. They considered 3, defined as *small*, to be the shelf-life limit, taking this limit from a previous paper (Djenane et al. 2001) where this limit is not even mentioned, let alone justified. Here again the SSL was centered on the product, as there was no indication of what consumers would think about a *small* off-odor. That is, there is a pork sausage on a plate that has no sanitary problems. A six-member panel decides that this sausage had a *small* off-odor. This gives no indication at all on the SSL of the sausage. The response of consumers to this sausage could be:

- Reject the sausage due to the off-odor
- Not detect the off-odor as such, considering it part of the general odor to be expected in a sausage. Thus, these consumers would accept this sausage, just as they accept the fresh sample.
- Like the sausage with the off-odor more than the fresh sample, because it brings back memories of homemade sausages consumed

on a farm during childhood. These consumers would probably reject the fresh sausage and accept this off-odor one.

In a more recent article (Sirpatrawan 2009) on the SSL of rice crackers, a 10-member trained panel measured acceptability using a scale of 1 (*extremely undesirable*) to 5 (*extremely desirable*). Chapter 2 (Section 2.3) noted that using a trained panel to measure acceptability is not good practice; thus, the sensory methodology was not adequate. To determine SSL these acceptability scores were regressed versus water activity values, and considering a limiting value of 3 on the acceptability scale, critical water activities were defined. Here again, SSL is centered on the product. A cracker that had reached the critical water activity based on the arbitrary value of acceptability = 3 would be considered to have reached the end of its shelf life. Some consumers would find this cracker acceptable, and others would find it unacceptable. Also, the same consumer may find the cracker unacceptable alone and okay if accompanied with butter and jam. In Argentina it is common to dunk this type of bulky cracker in an accompanying beverage like chocolate flavored milk or coffee with milk. What happens to the critical water activity in this case?

4.5 Experimental data used to illustrate the methodology

To illustrate the methodology to be applied to estimate SSL using survival analysis statistics, data from a yogurt storage test will be used. A commercial, whole-fat, stirred, strawberry-flavored yogurt with strawberry pulp was used. Pots (150 g) were bought from a local distributor, all from the same batch. A reversed storage design was used (see Chapter 3, Section 3.3.6.2). The pots were kept at 4°C, and some of them were periodically placed in a 42°C oven. This particularly high temperature was chosen with the sole purpose of generating data to illustrate the methodology. Samples were stored at 42°C for the following times: 0, 4, 8, 12, 24, 36, and 48 hours. These times were chosen because a preliminary experiment showed that the flavor deteriorated quickly up to approximately 12 hours and then the deterioration slowed down. Once samples had reached the storage time at 42°C, they were refrigerated at 4°C until they were tasted; this refrigerated storage lasted between 1 and 3 days. Previous microbiological analysis (aerobic mesophiles, coliforms, yeasts, and molds) showed that the samples were fit for consumption. The ethics committee of our institute (see Chapter 2, Section 2.6.9) decided that all samples were adequate for tests on humans in the quantities to be served.

Fifty subjects who consumed stirred yogurt at least once a week were recruited from the town of Nueve de Julio (Buenos Aires, Argentina). They were presented with the seven yogurt samples (0-, 4-, 8-, 12-, 24-,

36-, and 48-hour storage time at 42°C) monadically in random order. Fifty grams of each sample was presented in a 70-ml plastic cup. Time between each sample was approximately 1 minute. Water was available for rinsing. For each sample, subjects tasted the sample and answered the question: "Would you normally consume this product? Yes or No?" It was explained that this meant: If they had bought the product to eat it, or if it was served to them at their homes, would they normally consume it or not? The tests were conducted in a sensory laboratory with individual booths with artificial daylight-type illumination, temperature control (between 22 and 24°C) and air circulation. The data obtained from the 50 consumers are in Table 4.1.

4.6 Censoring in shelf-life data

Table 4.2 presents the data for 5 of the 50 subjects to illustrate the interpretation given to each subject's data:

- *Subject 1* was as expected in a shelf-life study; that is, the subject accepted the samples up to a certain storage time and then consistently rejected them. The data are interval-censored because we do not know at exactly what storage time between 12 and 24 hours the consumer would start rejecting the product. Twenty-two subjects presented this type of data.
- *Subject 2* accepted all samples. Supposedly at a sufficiently long storage time ($T > 48$ h) the sample would be rejected and thus the data are right-censored. Eight subjects presented this type of data.
- *Subject 3* was rather inconsistent, rejecting the sample with 8 hours' storage, accepting at 12 hours' storage, and rejecting from 24 hours' storage and onward. Censoring could be interpreted in different ways. One possibility would be to consider the data as interval-censored between 4 and 8 hours; that is, ignoring the subject's answers after the first time the yogurt is rejected. Another possibility, as shown in Table 4.2, is interval-censoring between 4 and 24 hours. We consider this option as more representative of the subject's data; that is, we assign a wider uncertainty interval as to the storage time at which this subject rejects the yogurt. Eleven subjects presented this type of data.
- *Subject 4* was also rather inconsistent, with alternating *no* and *yes* answers. This subject's data were considered left-censored. Left-censoring is a special case of interval-censoring with the lower bound equal to Time = 0 (Meeker and Escobar 1998). But as the literature and statistical software distinguish it, we have also done so. The left-censoring could be considered as $T \leq 4$ h or $T \leq 24$ hours. As with Subject 3, a wider interval is recommended for Subject 4, as this

Table 4.1 Consumer Acceptance/Rejection Data for Yogurt Stored at 42°C

Consumer	t0	t4	t8	t12	t24	t36	t48
1	no	no	yes	yes	yes	yes	no
2	yes	yes	no	yes	no	no	no
3	yes	yes	no	yes	no	no	yes
4	yes	no	yes	yes	no	no	no
5	yes	yes	yes	yes	yes	yes	no
6	yes	yes	yes	yes	no	yes	no
7	no	yes	yes	yes	yes	yes	no
8	yes	yes	yes	yes	yes	yes	yes
9	yes	yes	yes	yes	no	no	no
10	yes	yes	yes	yes	no	yes	no
11	yes	yes	no	yes	yes	no	no
12	yes	yes	yes	yes	yes	no	no
13	yes	yes	yes	no	no	no	no
14	yes	yes	yes	yes	yes	no	no
15	yes	yes	yes	no	no	no	no
16	yes	yes	yes	yes	yes	yes	no
17	no	yes	no	yes	no	yes	yes
18	yes	yes	no	no	no	no	no
19	yes	yes	yes	yes	no	no	no
20	yes	yes	no	yes	no	yes	no
21	yes	yes	yes	no	yes	yes	yes
22	yes	yes	yes	yes	no	no	no
23	yes	yes	no	no	no	no	no
24	yes	yes	yes	yes	yes	yes	no
25	yes	yes	yes	yes	yes	no	no
26	yes	no	no	yes	no	no	no
27	yes	yes	no	no	no	no	no
28	no	yes	yes	yes	no	no	no
29	yes	yes	yes	no	yes	no	no
30	yes	yes	no	yes	no	no	no
31	yes	yes	yes	yes	yes	no	no
32	yes	yes	yes	yes	yes	no	yes
33	yes	no	no	yes	yes	no	no
34	yes	yes	yes	no	no	no	no
35	yes	yes	yes	yes	no	no	no
36	yes	yes	yes	yes	yes	yes	yes
37	yes	yes	yes	yes	yes	yes	no

(continued on next page)

Table 4.1 (continued) Consumer Acceptance/Rejection Data for Yogurt Stored at 42°C

Consumer	t0	t4	t8	t12	t24	t36	t48
38	yes	no	yes	yes	yes	no	no
39	yes	yes	yes	no	no	no	no
40	yes	no	yes	yes	yes	no	no
41	yes	yes	yes	yes	no	no	yes
42	yes	yes	yes	yes	no	yes	no
43	yes	yes	no	no	no	no	no
44	yes	yes	no	no	no	no	no
45	yes	yes	yes	yes	yes	yes	yes
46	yes	yes	yes	yes	no	yes	no
47	yes	yes	no	yes	no	no	no
48	yes	no	no	no	no	no	no
49	yes	yes	yes	yes	no	no	no
50	yes	yes	yes	yes	yes	yes	yes

Note: The full data can be downloaded from the editor's Web site: yogur.xls.

Table 4.2 Acceptance/Rejection Data for Five Subjects Who Tasted Yogurt Samples with Different Storage Times at 42°C

	Storage time (hours)							
Subject	0	4	8	12	24	36	48	Censoring
1	yes	yes	yes	yes	no	no	no	Interval: 12–24
2	yes	yes	yes	yes	yes	yes	yes	Right: >48
3	yes	yes	no	yes	no	no	no	Interval: 4–24
4	yes	no	yes	yes	no	no	no	Left: ≤24
5	no	no	yes	yes	yes	yes	no	Not consider

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reflects the true uncertainty of the subject's response. Five subjects were left-censored.

- *Subject 5* rejected the fresh sample. This subject was either (a) recruited by mistake, that is, he did not like yogurt, or (b) he preferred the stored product to the fresh product, or (c) he did not understand the task. It would not be reasonable to consider the results of these subjects in establishing the shelf life of a product. For example, for consumers who preferred the stored to the fresh product, a company would have to produce a yogurt with a different flavor profile

Table 4.3 Sample of Data Ready to Be Processed to Maximize the Likelihood Function and Thus Obtain the Model's Parameters

Subject	Low time interval	High time interval	Type of censorship
1	12	24	Interval
2	48	48	Right
3	4	24	Interval
4	24	24	Left

rather than encourage them to consume an aged product. Four subjects presented this behavior of rejecting the fresh sample, and their results were not considered.

Table 4.3 presents the data from the consumers of Table 4.2 in a form ready to estimate to maximize the likelihood function and estimate the model's parameters as explained in the following section.

4.7 Model to estimate the rejection function

A simple way of estimating the rejection function is to calculate the experimental percent rejection corresponding to each storage time. For example, for a storage time of 4 hours corresponding to the yogurt data in Table 4.1, the experimental percent rejection = 6/46 × 100 = 13%. The total number of consumers who accepted the fresh sample was 46. Figure 4.3 presents the results of these calculations for each storage time. This figure can be used to obtain an approximate shelf-life value. If 50% rejection probability is considered, estimated shelf life is 24 hours. This value is not very reliable. Figure 4.3 shows that it covers a percent rejection between 25% and 60%. Also, confidence intervals cannot be estimated.

The likelihood function, which is generally used to estimate the rejection function, is the joint probability of the given observations of the n consumers (Klein and Moeschberger 1997):

$$L = \prod_{i\varepsilon R}\left(1 - F(r_i)\right)\prod_{i\varepsilon L} F(l_i)\prod_{i\varepsilon I}\left(F(r_i) - F(l_i)\right) \tag{4.1}$$

where R is the set of right-censored observations, L the set of left-censored observations, and I the set of interval-censored observations. Equation 4.1 shows how each type of censoring contributes differently to the likelihood function.

If we can assume an appropriate distribution for the data, the use of parametric models provides adequate estimates of the rejection function and other values of interest. Usually, rejection times are not normally

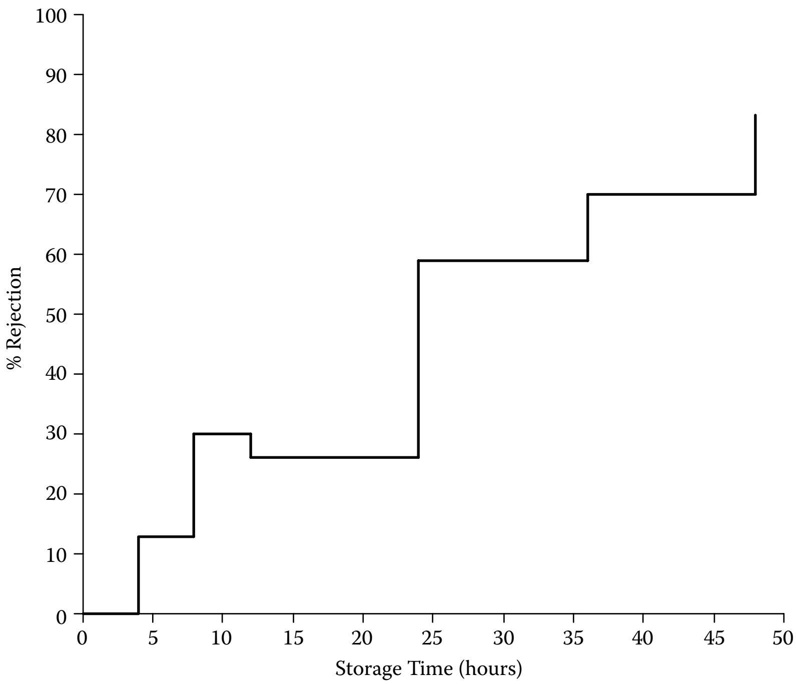


Figure 4.3 Experimental percent rejection versus storage time for the yogurt data.

distributed; instead, their distribution is often right-skewed. Often, a log-linear model is chosen:

$$Y = \ln(T) = \mu + \sigma W$$

where W is the error term distribution. That is, instead of the rejection time T, its logarithmic transformation is modeled. In Klein and Moeschberger (1997) or Meeker and Escobar (1998) different possible distributions for T are presented, for example, the log-normal or the Weibull distribution. With the former, W is the standard normal distribution; and with the latter, W is the smallest extreme value distribution.

If the log-normal distribution is chosen for T, the rejection function is given by:

$$F(t) = \Phi\left(\frac{\ln(t) - \mu}{\sigma}\right) \quad (4.2)$$

where $\Phi(\cdot)$ is the standard normal cumulative distribution function, and μ and σ are the model's parameters.

If the Weibull distribution is chosen, the rejection function is given by:

$$F(t) = F_{sev}\left(\frac{\ln(t)-\mu}{\sigma}\right)$$

where $F_{sev}(\cdot)$ is the rejection function of the extreme value distribution:

$$F_{sev}(w) = 1-\exp\left(-\exp(w)\right)$$

Thus the rejection function for the Weibull distribution can be expressed as:

$$F(t) = 1-\exp\left[-\exp\left(\frac{\ln(t)-\mu}{\sigma}\right)\right] \quad (4.3)$$

where μ and σ are the model's parameters. Some authors express the Weibull rejection function in another manner (Meeker and Escobar 1998; Gacula and Singh 1984):

$$F(t) = 1-\exp\left(-\left(\frac{t}{\eta}\right)^{\beta}\right)$$

The relationship between β and η of this last equation and μ and σ from Equation 4.3 is the following:

$$\sigma = 1/\beta$$

and

$$\mu = \ln(\eta)$$

Thus, either of the two expressions can be used. We prefer using Equation 4.3, as μ and σ are the parameters calculated by the statistical packages we use.

The parameters of the loglinear model are obtained by maximizing the likelihood function (Equation 4.1). The likelihood function is a mathematical expression that describes the joint probability of obtaining the data actually observed on the subjects in the study as a function of the unknown parameters of the model considered. To estimate μ and σ for the log-normal or the Weibull distribution, we maximize the likelihood function by substituting F(t) in Equation 4.1 by the expressions given in Equations 4.2 or 4.3, respectively.

Once the likelihood function is formed for a given model, specialized software can be used to estimate the parameters (μ and σ) that maximize the likelihood function for the given experimental data. The maximization is obtained by numerically solving the following system of equations using methods like the Newton-Raphson method (Gómez and Langohr 2002):

$$\frac{\partial \ln L(\mu,\sigma)}{\partial \mu} = 0$$

$$\frac{\partial \ln L(\mu,\sigma)}{\partial \sigma} = 0$$

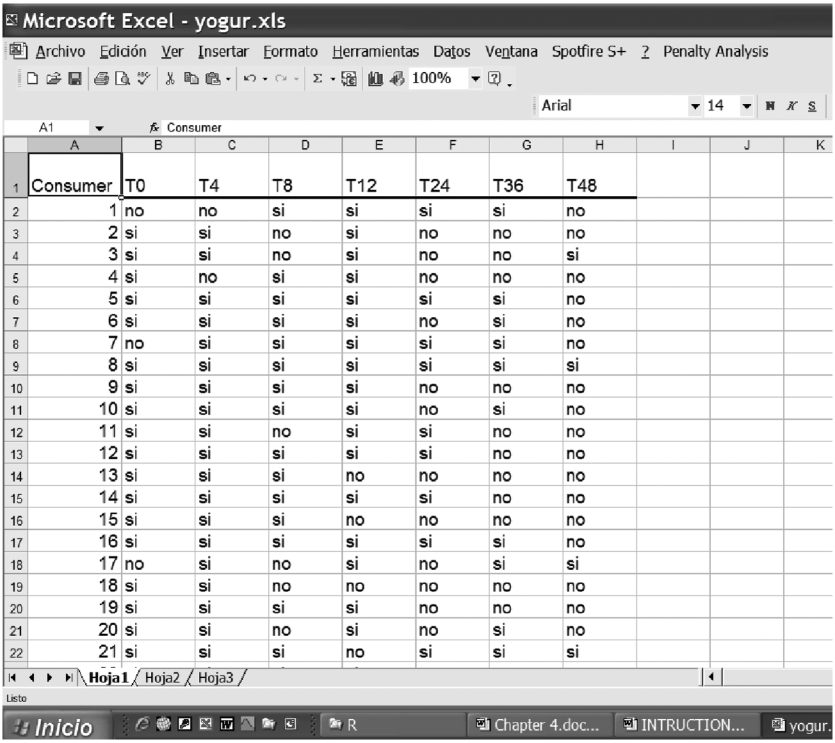
For more details on likelihood functions see Klein and Moeschberger (1997) or Meeker and Escobar (1998). In practice the numerical maximization of the likelihood function is performed with specialized software such as TIBCO Spotfire S+ (TIBCO, Inc.; Seattle, WA) or the R Statistical Package (http://www.r-project.org/; accessed May 26, 2009), as will be illustrated in the following sections.

4.8 Calculations using the R statistical package

As mentioned in Section 4.6, one of the characteristics of SSL data is the presence of interval-censored data. Not all statistical software has the necessary procedures to deal with this type of censoring. Commercial software such as TIBCO Spotfire S+ (TIBCO, Inc., Seattle, WA) and SAS (SAS Institute, Inc., Cary, NC) have interval-censoring procedures. R, a free-access statistical package that can be downloaded from http://www.r-project.org (accessed May 26, 2009), does have a procedure for interval-censoring calculations and shall be used in the present book.

The first step in performing calculations is to have the raw data in an Excel spreadsheet, as shown in Figure 4.4 for the first 21 of the 50 consumers of Table 4.1. For this Excel spreadsheet to be compatible with the function written in R for SSL calculations, the spreadsheet should have the following characteristics:

1. The first column should indicate the consumer number. These numbers do not necessarily have to be consecutive nor start from 1, but all cells should be numbered and the column should have a text heading. In this example the heading is *consumer*, but it could be any other name.
2. The first row should contain label headings for each column, starting with the *consumer* column and following with the storage time



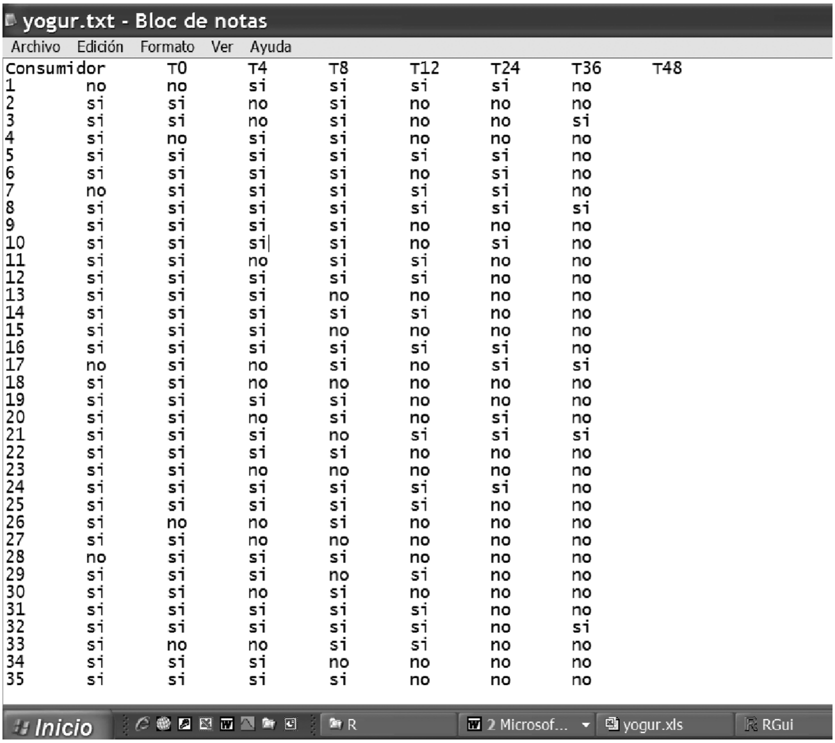
Consumer	T0	T4	T8	T12	T24	T36	T48
1	no	no	si	si	si	si	no
2	si	si	no	si	no	no	no
3	si	si	no	si	no	no	si
4	si	no	si	si	no	no	no
5	si	si	si	si	si	si	no
6	si	si	si	si	no	si	no
7	no	si	si	si	si	si	no
8	si	si	si	si	si	si	si
9	si	si	si	si	no	no	no
10	si	si	si	si	no	si	no
11	si	si	no	si	si	no	no
12	si	si	si	si	si	no	no
13	si	si	si	no	no	no	no
14	si	si	si	si	si	no	no
15	si	si	si	no	no	no	no
16	si	si	si	si	si	si	no
17	no	si	no	si	no	si	si
18	si	si	no	no	no	no	no
19	si	si	si	si	no	no	no
20	si	si	no	si	no	si	no
21	si	si	si	no	si	si	si

Figure 4.4 Excel spreadhsheet showing raw data from a storage study of yogurt.

columns. What these columns actually say is not important. In the present example the labels are T0, T4, T8, T12, T24, T36, and T48; but they could have been time0, time4 or t1, t2, t3, and so forth. The actual storage times will be provided when using the corresponding function within R.

3. The answers of acceptance or rejection for each one of the samples by consumers can be coded as wished. In the present example the codes are *no* for rejection and *si* (*yes* in Spanish) for acceptance. The codes could be numerical, for example a 0 for rejection and a 1 for acceptance or other labels such as *rej* for rejection and *acc* for acceptance.

The data in the format shown in Figure 4.4 should be saved as a tab-delimited text file (extension *txt*) as shown in Figure 4.5. This format can be easily read by R. Once R has been installed, the instructions to analyze the yogurt data saved in the text file shown in Figure 4.5 would be as follows:



Consumidor	T0	T4	T8	T12	T24	T36	T48
1	no	no	si	si	si	si	no
2	si	si	no	si	no	no	no
3	si	si	no	si	no	no	si
4	si	no	si	si	no	no	no
5	si	si	si	si	si	si	no
6	si	si	si	si	no	si	no
7	no	si	si	si	si	si	no
8	si	si	si	si	si	si	si
9	si	si	si	si	no	no	no
10	si	si	si	si	no	si	no
11	si	si	no	si	si	no	no
12	si	si	si	si	si	no	no
13	si	si	si	no	no	no	no
14	si	si	si	si	si	no	no
15	si	si	si	no	no	no	no
16	si	si	si	si	si	si	no
17	no	si	no	si	no	si	si
18	si	si	no	no	no	no	no
19	si	si	si	si	no	no	no
20	si	si	no	si	no	si	no
21	si	si	si	no	si	si	si
22	si	si	si	si	no	no	no
23	si	si	no	no	no	no	no
24	si	si	si	si	si	si	no
25	si	si	si	si	si	no	no
26	si	no	no	si	no	no	no
27	si	si	no	no	no	no	no
28	no	si	si	si	no	no	no
29	si	si	si	no	si	no	no
30	si	si	no	si	no	no	no
31	si	si	si	si	si	no	no
32	si	si	si	si	si	no	si
33	si	no	no	si	si	no	no
34	si	si	si	no	no	no	no
35	si	si	si	si	no	no	no

Figure 4.5 Raw data from a storage study of yogurt in shown text format.

1. Open R.
2. Go to the File Menu and change the directory to where the yogur.txt file was saved.
3. Go to the File Menu and open a New Script. This will bring up an empty window.
4. Introduce the text shown in Figure 4.6 in the New Script window. Once it has been introduced, save this window as “sslife.R”
5. What is sslife.R? It is a function for analyzing shelf-life data in a format such as shown in Table 4.1. The sslife.R function has the following format and options:

```
sslife <- function(data, tiempos = c(0, 4, 8, 12,
24, 36, 48), codiresp = c("si," "no"),model="weibu
ll,"percent=c(10,25,50))
```

```
sslife <- function(data, tiempos = c(0, 4, 8, 12, 24, 36, 48), codiresp =
c("si", "no"),model="weibull",percent=c(10,25,50))
{
   library(survival)
   totalcases <- dim(data)[1]
        casesdata <- cbind(1:totalcases, data)
        casesok <- casesdata[, 1][data[, 2] == codiresp[1]]
        numindok <- length(casesok)
        numtimes <- length(tiempos)
        id <- data[casesok, 1]
        respcod <- data[casesok, 2:dim(data)[2]]
        respnum <- matrix(rep(1, numindok * numtimes), ncol = numtimes)
        respnum[respcod == codiresp[2]] <- 0
        ti <- rep(tiempos[1], numindok)
        ts <- rep(tiempos[numtimes], numindok)
        cens <- rep("interval", numindok)
        censcod <- rep(3, numindok)
        for(i in 1:numindok) {
                  if(respnum[i, numtimes] == 1) {
                         ti[i] <- tiempos[numtimes]
                         ts[i] <- tiempos[numtimes]
                         cens[i] <- "right"
                         censcod[i] <- 0
                  }
                  else {
                         inf <- 1
                         while(respnum[i, inf + 1] == 1) inf <- inf + 1
                         sup <- numtimes
                         while(respnum[i, sup - 1] == 0) sup <- sup - 1
                         if(inf == 1) {
                                  ti[i] <- tiempos[sup]
                                  ts[i] <- tiempos[sup]
                                  cens[i] <- "left"
                                  censcod[i] <- 2
                         }
                         else {
                                  ti[i] <- tiempos[inf]
                                  ts[i] <- tiempos[sup]
                         }
                  }
        }
        prop<-percent/100
   pp1<-data.frame(id, ti, ts, cens, censcod)
   pp2<-survreg(Surv(ti,ts,censcod,type="interval")~1,dist=model)
     pp4<-predict(pp2,newdata=data.frame(1),type = "uquantile", p =
      prop, se.fit = T)
       ci3 <- cbind(pp4$fit,pp4$fit - 1.96 * pp4$se.fit,pp4$fit + 1.96 *
        pp4$se.fit)
   if (model=="weibull"|model=="lognormal"|model=="loglogistic"|model==
    "exponential") {
   ci3 <- exp(ci3)
   pp4$se.fit<-pp4$se.fit*ci3[,1]}
   ci2<-cbind(ci3,pp4$se.fit)
   mu <- c(pp2$coefficients,pp2$coefficients - 1.96 * sqrt(pp2$var[1,1]),
    pp2$coefficients + 1.96 * sqrt(pp2$var[1,1]))
```

Figure 4.6 R-function for estimating sensory shelf life.

```
   if (model==»exponential») {
   sigma<-c(NA,NA,NA)}
   else {
   si<-exp(pp2$icoef[2])
   sigma<-c(si,exp(log(si)-1.96*sqrt(pp2$var[2,2])),exp(log(si)+1.96*
sqrt(pp2$var[2,2])))
   }
   dimnames(ci2) <- list(percent, c("Estimate","Lower ci", "Upper ci",
"Serror"))
   value<-c(«estimate»,»lower»,»upper»)
   list(censdata=pp1,musig=data.frame(value,mu,sigma),loglike=-
pp2$loglik[1],slives=ci2)
}
```

Figure 4.6 (continued).

- data: raw data of acceptance/rejection; no default, must be introduced.
- tiempos: food storage times; default values: c(0, 4, 8, 12, 24, 36, 48)
- codiresp: codes for consumer responses of acceptance ("si") or rejection ("no"); default values: c("si")("no").
- model: parametric model of choice (weibull, exponential, gaussian, logistic, log-normal or loglogistic); default: weibull.
- percent: percent rejection values for which estimated shelf lives are wanted; default values: c(10,25,50). For example, if estimated shelf lives are wanted for percent rejections = 10%, 20%, 30%, 40% and 50%, then percent = c(10,20,30,40,50). If a table with estimated shelf lives for a sequence of percent rejections from 10% to 50% at 1% increments is wanted, then percent = c(seq(10,50,by=1)).

6. Caveat: When text is copied from Word and pasted into R, the quotation marks are sometimes not read properly and have to be retyped in R.
7. Instructions in R are written in the R Console window after the > symbol; thus, to read the raw data the following instruction has to be written:

```
> yog <-read.table("yogurt.txt",=Header=True)
```

- <- ("less than" symbol followed by a hyphen) is supposed to symbolize an arrow and is equivalent to an equal or assignment symbol.
- Alternatively you could read the data from a directory other than the working directory; for example:

```
> yog<- read.table("C:\HOUGH\R_FILES\yogur.txt",
Header=TRUE)
```

8. Go to the File Menu, Open Source R-code: sslife.R.
9. For the yogur.txt data, use sslife with default options except for the model:

```
> resyog <- sslife(yog, model= "lognormal")
```

10. After executing the previous instruction by pressing Enter, the following message appears: "Loading required package: splines."
11. The results of the SSL analysis are in a data structure called *resyog*, which contains the censored data, the model's parameters, the log-likelihood value, and estimated storage times corresponding to different percent rejections.
12. To view the censored data:

```
> resyog$censdata
```

	id	ti	ts	cens	censcod
1	2	4	24	interval	3
2	3	48	48	right	0
3	4	24	24	left	2
4	5	36	48	interval	3
…	…	…	…	…	…
42	46	12	48	interval	3
43	47	4	24	interval	3
44	48	4	4	left	2
45	49	12	24	interval	3
46	50	48	48	right	0

13. The previous table corresponds with the data in Table 4.1 transformed according to the guidelines described in Section 4.6. The first column indicates the number of resulting rows. Note that there are 46 rows and not 50; this is because 4 consumers rejected the fresh sample, as can be seen in Table 4.1. The second column indicates the consumer number corresponding to Table 4.1. The third and fourth columns are the low and high time intervals corresponding to each consumer's rejection time; for right- and left-censored data the corresponding time is repeated. The fifth column indicates the type of censoring corresponding to each consumer, and the sixth column is

the code R used to interpret each type of censoring: 0, 2, and 3 for right-, left-, and interval-censored data, respectively.

14. To list the model's parameters:

```
> resyog$musig
```

	value	mu	sigma
1	estimate	2.987802	0.9292777
2	lower	2.695269	0.7129343
3	upper	3.280336	1.2112717

15. The previous table shows the model's parameters—in this case the μ and σ values corresponding to the log-normal distribution expressed in Equation 4.2. Row 1 is the mean estimate of each parameter, and rows 2 and 3 correspond to the lower and upper 95% confidence intervals, respectively. If $\mu = 2.988$ and $\sigma = 0.929$ are introduced in Equation 4.2, percent rejection versus storage time can be graphed as shown in Figure 4.7. The Excel function for the log-normal distribution is DISTR.LOG.NORM(t, μ, σ).
16. To list the loglikelihood:

```
> resyog$loglike
[1] 66.7457
```

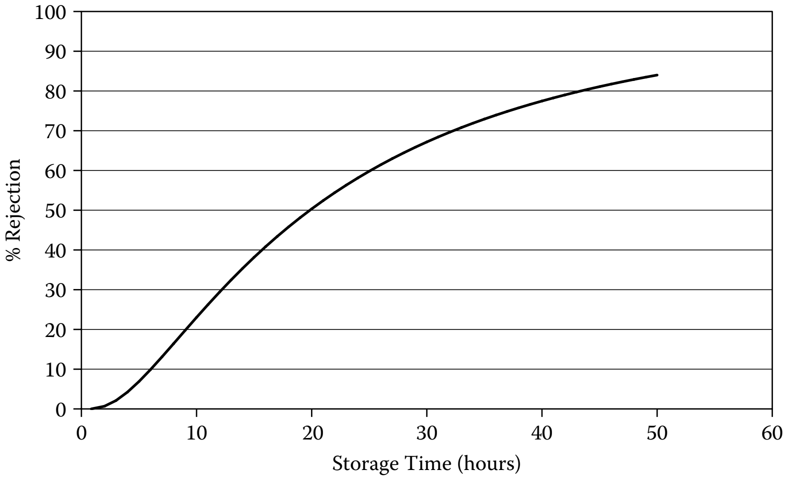


Figure 4.7 Percent rejection versus storage time corresponding to the yogurt data (Table 4.1) for the log-normal model.

17. To compare which model best fits the data, TIBCO Spotfire S+ offers the possibility of producing a graph that compares the fit of different distributions with the experimental data, and thus a visual comparison defines which is the most adequate distribution. R does not produce this graph, and thus a way to define the best fit is to compare the loglikelihood values; the model that gives the lowest loglikelihood would be the best. In actual fact, the loglikelihood is to be used when comparing models contained one in another (Meeker and Escobar 1998); thus the criteria for choosing different models based on the loglikelihood are only approximate. In all the data we have processed, the criteria of choosing the model with the lowest loglikelihood coincided with the criteria of visual examination performed with the TIBCO Spotfire S+ software. For the present yogurt data the log-normal distribution had the lowest loglikelihood value.
18. To list the predicted shelf lives with their confidence intervals and standard errors:

```
>resyog$slives
```

percent	estimate	lower ci	upper ci	serror
10	6.030833	3.910189	9.301583	1.333243
25	10.601698	7.558044	14.871042	1.830425
50	19.842031	14.809504	26.5847	2.961457

19. In the first column of the previous table are the percent rejection values, in this case 10%, 25%, and 50%. In the second column are the estimated storage times corresponding to each percent rejection. In the third and fourth columns are the lower and upper 95% confidence limits, respectively. In the fifth column are the standard errors of the estimations.
20. Instead of listing the structures contained in *resyog* separately, they can all be listed together by simply typing:

```
> resyog
```

4.9 Interpretation of shelf-life calculations

After calculations have been performed, an SSL value has to be recommended. To do this an adequate percent rejection has to be adopted. What can be considered *adequate*? Gacula and Singh (1984) mentioned a nominal shelf-life value considering 50% rejection, and Cardelli and Labuza (2001) used this criterion in calculating the shelf life of coffee. Curia et al. (2005)

estimated SSL values of yogurt for 25% and 50% rejection probabilities. This means that if a consumer tastes a product with a storage time corresponding to 50% rejection probability, there is a 50% probability that the consumers will reject the product. This can sound too risky, yet it must be remembered that we are referring to a consumer who tastes the product at the end of its shelf life. Distribution times usually guarantee that the proportion of consumers who taste the product close to the end of its SSL is small. Of this small proportion of consumers, 50% will reject the product and 50% will accept it.

How does this 25%–50% criterion compare with values used in studies of other types of food? In determining thresholds from forced-choice data sets, the threshold value is estimated for 50% probability detection above chance (ASTM Standard E1432-04 2006; ISO Standard 13301 2002). The ISO Standard 4120 (2004) for the triangle test establishes three categories for the maximum allowable proportion of distinguishers, p_d:

- $p_d < 25\%$ represents small values
- $25\% < p_d < 35\%$ represents medium size values
- $p_d > 35\%$ represents large values

Thus, considering percent rejection, a probability in the range of 25% to 50% is in line with international sensory analysis standards where criteria are established to decide when the proportion of the population who can tell a difference is important.

We have had a number of clients with product on the market with a *best before* date stamped on it based on commercial experience and not on an SSL study. Their objective when conducting an SSL test was to confirm if this *best before* date was adequate. In this case, once the model's parameters μ and σ had been calculated, it was in their interest to estimate the percent rejection for their current *best before* date. If, for example, the lognormal model was chosen to model percent rejection, Equation 4.2 can be used to this purpose replacing t in the right side of the equation and calculating $F(t)$. Likewise, if the Weibull model was chosen, Equation 4.3 can be used.

An important aspect of survival analysis methodology is that experimental sensory work is relatively simple. In the above yogurt example 50 consumers each tasted seven yogurt samples with different storage times, answering *yes* or *no* to whether they would consume the samples. This information was sufficient to model the probability of consumers accepting the products with different storage times, and from the model shelf-life estimations were made. There was no necessity to have a trained sensory panel.

Another important aspect is that the information obtained from consumers by this method is directly related to their everyday eating experience. When consumers are confronted with a food product, they either

accept or reject it. They do not mentally assign the product a hedonic score of 8 on a 1–9 scale and thus decide the product is acceptable, nor assign the product a score of 4 and thus decide to reject the product. Survival analysis methodology taps into direct consumer experience.

4.10 An additional example

SSL of fat-free stirred strawberry yogurt was studied at a storage temperature of 10°C. Yogurts were obtained from a dairy company. Bottles (1000 ml) from different batches were stored at 10°C in such a way as to have samples with different storage times ready on the same day. Storage times at 10°C were 0, 14, 28, 42, 56, 70, and 84 days. All batches were made with the same formulation and were checked to be similar to the previous batch by consensus among three expert assessors. Storage times were chosen based on a preliminary experiment. Once samples had reached the storage time at 10°C, they were refrigerated at 2°C, until they were tasted. All the measurements were made in a period not longer than a week, to guarantee no changes in the samples. To ensure that the samples were fit for consumption, the following microbiological analysis were performed on samples from the different batches and on the yogurts stored for 80 days at 10°C: coliforms, yeasts, molds, and *Staphylococcus aureus*, using standard methods of analysis (Elliott et al. 1982).

Eighty people who consumed fat-free stirred yogurt at least once a week were recruited from the city of Nueve de Julio, Buenos Aires, Argentina. Each consumer received the seven yogurt samples (corresponding to each storage time at 10°C) monadically in random order. Fifty grams of each sample were served in 70-ml plastic cups. Water was available for rinsing. For each sample subjects had to answer the question: "Would you normally consume this product: yes or no?" The data for 10 of these consumers is in Table 4.4. Of the 80 consumers, 6 rejected the fresh sample, so their data were not considered; 2 were right-censored, 18 left-censored, and 54 interval-censored. As mentioned in Section 4.8, to process the data with R, the data must be stored in a tab-delimited text file. Suppose we store this data in "strawberry.txt."

1. In the 'R Console' window write the following instruction:

   ```
   > straw <-read.table("strawberry.txt",header=TRUE)
   ```

   Alternatively you could read the data from a directory other than the working directory, for example:

   ```
   > yog<- read.table("C:\HOUGH\R_FILES\strawberry.
   txt",header=TRUE)
   ```

Table 4.4 Acceptance/Rejection Data for 10 Consumers Who Evaluated Fat-Free Stirred Yogurt Stored at 10°C

Consumer	t0	t14	t28	t42	t56	t70	t84
1	0	0	1	0	1	1	1
2	0	0	1	0	0	1	1
3	0	0	1	0	0	1	1
4	0	1	0	1	0	1	1
5	0	0	1	1	1	1	1
6	0	1	1	0	0	1	1
7	0	1	0	1	0	1	1
8	0	0	0	0	1	1	1
9	0	0	1	0	0	1	1
10	0	0	1	0	1	1	1

Note: Acceptance is symbolized by 0 and rejection by 1. The full data can be downloaded from the editor's Web site: strawberry.xls.

2. Go to the File Menu, Open Source R-code: sslife.R.
3. For the strawberry data, sslife has to receive the data (straw), the time points (c(0,14,28,42,56,70,84)), the response codes (c("0","1")) and the model ("log-normal"):

```
> resstraw<-sslife(straw,c(0,14,28,42,56,70,84),
c("0","1"),model="lognormal")
```

4. The results of the SSL analysis are in a data structure called *resstraw*, which contains the censored data, the model's parameters, the log-likelihood value, and estimated storage times corresponding to different percent rejections (in this case we adopted the default values of 10%, 25%, and 50%). The first step will be to choose the most adequate model. To do this type:

```
> resstraw$loglike
[1] 92.78819
```

5. Repeat Steps 3 and 4 for the other possible models: exponential, Gaussian, logistic, loglogistic, and Weibull. The resulting loglikelihood values are in Table 4.5. The logistic distribution gives a slightly lower loglikelihood value than the Gaussian (or normal) distribution. The shape of the logistic distribution is very similar to that of the normal distribution; in fact, it would require an extremely large number of observations to assess whether data come from a normal or logistic distribution (Meeker and Escobar 1998). The loglikelihood

Table 4.5 Loglikelihood Values for Different Models Corresponding to the Fat-Free Strawberry Yogurt Data

Model	Loglikelihood
Logistic	83.6
Gaussian	84.1
Weibull	84.9
Loglogistic	90.3
Log-normal	92.8
Exponential	116

values for these two distributions have always been very similar for SSL data we have processed. Thus, the logistic function would rarely need to be considered. The hazard function corresponding to the exponential function is constant, that is, it would correspond to elements or populations that do not age. Certain electronic components behave in this manner, but not food. If a yogurt has been stored for 10 days at 10°C and was accepted by the consumer, the probability of this consumer rejecting the yogurt on the following day is low. However, if a consumer accepts a yogurt stored for 40 days, the probability of this consumer rejecting the yogurt on the following day is high. This occurs because the product has aged. Thus the exponential function would not be adequate for SSL studies of food products. In all cases that we have tested it, its loglikelihood has been higher than other models. Going back to Table 4.5, the choice would be between the normal and Weibull distributions. We shall choose the normal distribution.

6. Calculations for the normal or Gaussian distribution are performed with the following instruction in R:

```
> resstraw<-sslife(straw,c(0,14,28,42,56,70,84),
c("0","1"),model="gaussian")
```

7. To obtain the censored data:

```
> resstraw$censdata
```

	id	ti	ts	cens	censcod
1	1	14	56	interval	3
2	3	14	70	interval	3
3	4	14	70	interval	3
4	5	70	70	left	2
…	…	…	…	…	…
70	76	42	56	interval	3
71	77	42	42	left	2
72	78	28	42	interval	3
73	79	42	56	interval	3
74	80	28	42	interval	3

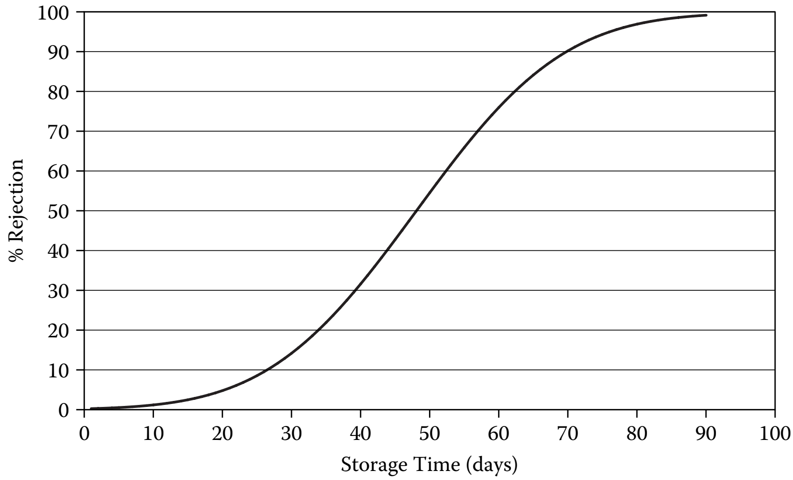


Figure 4.8 Percent rejection versus storage time corresponding to the fat-free stirred strawberry yogurt data for the normal model.

8. To list the models parameters:

```
> resstraw$musig
```

	value	mu	sigma
1	estimate	48.03002	16.84253
2	lower	43.53564	13.74913
3	upper	52.5244	20.63189

9. With the values of the previous table the percent rejection versus storage time curve can be drawn as shown in Figure 4.8. The Excel function for the cumulative normal distribution is =DISTR. NORM(t,μ,σ,TRUE)*100.
10. To list the predicted shelf lives with their confidence intervals and standard errors:

```
>resstraw$slives
```

percent	estimate	lower ci	upper ci	serror
10	26.44545	19.66408	33.22683	3.459885
25	36.66991	31.28582	42.054	2.746984
50	48.03002	43.53564	52.5244	2.293051

11. In this study the company had been using a *best before* date corresponding to 35 days' shelf life. The previous table shows that this corresponds to approximately 25% rejection probability, which was considered acceptable, and thus the company maintained the 35 days' shelf life with renewed confidence.
12. As shown in Table 4.5 the normal and Weibull distributions had similar loglikelihood values. What would have been the results if the Weibull distribution had been chosen? Calculations can be performed with the following instruction in R:

```
> resweib<-sslife(straw,c(0,14,28,42,56,70,84),
c("0","1"),model="weibull")
```

13. To list the model's parameters:

```
> resweib$musig
```

	value	mu	sigma
1	estimate	3.981363	0.3098097
2	lower	3.896379	0.2443884
3	upper	4.066348	0.392744

14. With the values of the previous table the percent rejection versus storage time curve can be drawn using Equation 4.3. This will not be done as the curve virtually superimposes the normal distribution curve shown in Figure 4.8.
15. To list the predicted shelf lives with their confidence intervals and standard errors:

```
>resweib$slives
```

percent	estimate	lower ci	upper ci	serror
10	26.68703	21.53232	33.07574	2.922265
25	36.42923	31.41094	42.24926	2.754782
50	47.8377	43.32459	52.82093	2.418575

16. These shelf-life values estimated using the Weibull distribution are very similar to those obtained using the normal distribution (see Step 10, above). Thus in practice, when the loglikelihood values are similar, final results do not differ. In these cases we tend to prefer the Weibull distribution as it is very flexible and right-skewed

and thus particularly appropriate for modeling survival data and it has been used previously in food shelf-life modeling (Cardelli and Labuza 2001; Duyvesteyn et al. 2001; Hough et al. 1999)

4.11 Should consumers be informed?

For SSL studies based on survival analysis statistics, samples with different storage times are presented to consumers. A practical question is whether consumers should be informed that they are evaluating samples with different storage times. Arguments *against* telling them would be as follows:

- If they are told they will pay special attention to samples, while in a natural setting they would not. The effect of this would be a shorter *best before* date than really necessary.
- They feel they are expected to find a sample that should be rejected.

Consider the case of a person who decides to open a carton of UHT milk on June 5, 2009. Supposing the *best before* date on the carton is October 5, 2009. In this case the person will be predisposed to thinking the milk is okay and will probably pay little attention to its sensory properties. If, however, the *best before* date is June 6, 2009 this will strike an alarm that the product may be of doubtful quality and now the person will pay attention to its sensory properties. With milk, the person was probably going to prepare a pudding or white sauce where any slight off-flavor would go unnoticed, but knowing the product is close to its *best before* date will lead the person to taste the milk on its own to see whether it is okay. It is for these consumers who taste the product close to its *best before* date and who thus pay special attention to its sensory properties that we are going to the trouble of estimating SSL. It is our policy to inform consumers that they are going to be evaluating samples with different storage times.

4.12 Is there a way to deal with totally new products?

In the experiments described in Sections 4.5 and 4.10 dealing with SSL of yogurts, regular consumers of the yogurts were recruited. When presented with the test samples, it was implied that they compare these to their internal reference of an acceptable product, and based on this comparison would tick either the *accept* or the *reject* box.

But what happens when the objective is to measure the SSL of a product that is new to the market? On one occasion we were asked to determine the SSL of canola oil, which was a product totally new to the

Argentine market. Canola oil has a distinct flavor. If an Argentine consumer were presented with a sample of stored canola oil and found that it had an odd flavor, she would not know whether this odd flavor was due to prolonged storage or was the typical flavor of canola oil. Because there was no internal reference, we presented consumers with a sample labeled *canola oil* and informed them that this was a fresh sample of the product with acceptable sensory properties. After this they were asked to evaluate the stored samples and tick one of two boxes labeled with *accept* or *reject*. This solution is not very satisfactory. In all probability consumers performed a discrimination task rather than an acceptability evaluation. That is, if they found a sensory difference between a stored sample and the "acceptable" control, they would most probably tick the *reject* box. For totally new products the safest approach is to conduct a discrimination test as described in Section 2.7.1.2. The resulting *best before* date would probably be too conservative. Once the product has been established on the market a consumer-based SSL determination can be made.

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